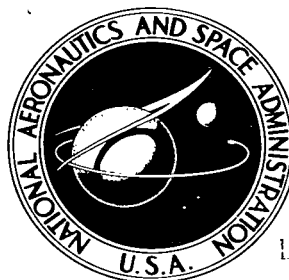


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NUMERICAL INTEGRATION OF DIFFERENTIAL EQUATIONS BY POWER SERIES EXPANSIONS, ILLUSTRATED BY PHYSICAL EXAMPLES

by Erwin Fehlberg

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Huntsville, Ala.*



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SUMMARY

Some general situations are discussed, where a power series expansion (with coefficients obtained by recurrence formulas) has advantages over other integration procedures.

Two examples are presented: the restricted problem of three bodies, and the motion of an electron in the field of a magnetic dipole. In these examples, the power series expansion requires only about 15 to 20 per cent of the computer time required by the Runge-Kutta-Nyström method, both methods yielding results of the same accuracy.

SECTION I. GENERAL REMARKS

1. Either a Runge-Kutta method or an interpolation procedure (Adams, Gauss, etc.) is generally used for the numerical solution of ordinary differential equations. Both methods have disadvantages in certain situations, however. Runge-Kutta formulas are of rather low accuracy (truncation errors proportional to h^5 for the Kutta formulas generally used). Runge-Kutta formulas therefore require integration step sizes that could be prohibitively small, resulting in excessive round-off errors and inordinately long computation times. Interpolation formulas, on the other hand, can be of any desired order of accuracy with respect to the truncation error. Interpolation formulas are well-suited for problems that can be integrated with a constant step size. But if the step size must be changed, reconstruction of the difference scheme, which is rather extensive for formulas of higher accuracy, is cumbersome. Thus our examples in II and III, which require frequent changes in the step size, could scarcely be integrated using an interpolation formula.

2. In such situations, numerical integration by power series expansions is preferable for some types of differential equations. For simplicity, let us consider a system of first order differential equations for the functions $y_\rho(x)$ for $\rho = 1, 2, \dots, n$. Clearly, such a system can always be solved by a power series expansion, with coefficients computed by recurrence formulas, provided the system is of second degree, i. e., that it has the form:

$$\frac{dy_\rho}{dx} \sum_{\nu=0}^n A_\nu y_\nu = \sum_{\mu, \nu}^{0 \dots n} B_{\mu, \nu} y_\mu y_\nu \quad (\rho = 1, 2, \dots, n) \quad (1)$$

where $y_0 \equiv 1$, and A_ν and $B_{\mu, \nu}$ can be polynomials of any degree in the independent variable x . Since we shall be concerned only with computational techniques, we shall assume that the power series expansions are sufficiently convergent for our purposes.

3. Differential equations of the simple form (1) are generally not encountered in practice. But a given system can in many cases be transformed into a system of form (1) through the introduction of suitable auxiliary functions, thus allowing solution by power series expansions (see II and III below). Indeed, since most of the common algebraic and transcendental functions satisfy differential equations of the simple form (1), a rather broad class of differential equations can be transformed into form (1) by suitable substitutions.

4. Another question arises, of course, as to how extensive the system will be after it has been transformed into form (1) by such substitutions. Integration of differential equations by power series expansion is recommended only if the equations can be transformed into form (1) by a small number of substitutions and, further, only if frequent changes in the integration step size are anticipated.

5. Like interpolation methods and unlike Runge-Kutta methods, the power series method permits computation of the truncation error along with the actual integration. This is fundamental to an automatic step size control. In the two examples that follow, we have made use of such an automatic step size control. These two examples, which involve systems of second order differential equations, were integrated both by power series methods and, for comparison, by the Runge-Kutta-Nyström method. Using the power series expansion method, we generally went as far as the terms with h^{16} , unless the coefficients exceeded the capacity of the computer in the neighborhood of singularities. To compare our power series method with the Runge-Kutta-Nyström method (truncation errors proportional to h^5), permissible tolerances of the truncation errors were adjusted so that the first integrals of the equations of motion (known in both examples) produce errors of approximately equal magnitude for both methods. Consequently, since our power series method is far more accurate than the Runge-Kutta-Nyström method, the step size will be much larger for our method. As our examples show, this larger step size can more than compensate for the considerably larger number of operations per integration step.

The computation of these examples was performed on an IBM 7090 computer in double precision (16 decimal places).¹

SECTION II. RESTRICTED PROBLEM OF THREE BODIES

6. The equations of motion (in a rotating coordinate system) are²

$$\left. \begin{aligned} \frac{d^2x}{dt^2} &= x + 2 \frac{dy}{dt} - (1 - \mu) \frac{x + \mu}{[(x+\mu)^2 + y^2]^{3/2}} - \mu \frac{x - (1-\mu)}{[(x-1+\mu)^2 + y^2]^{3/2}} \\ \frac{d^2y}{dt^2} &= y - 2 \frac{dx}{dt} - (1 - \mu) \frac{y}{[(x+\mu)^2 + y^2]^{3/2}} - \mu \frac{y}{[(x-1+\mu)^2 + y^2]^{3/2}} \end{aligned} \right\} \quad (2)$$

where μ = the relative mass of the Moon in the Earth-Moon system.

The first integral of the equations of motion (the so-called Jacobi integral) is

$$J = \frac{1}{2} \left[\left(\frac{dx}{dt} \right)^2 + \left(\frac{dy}{dt} \right)^2 - x^2 - y^2 \right] - \frac{1 - \mu}{[(x + \mu)^2 + y^2]^{1/2}} - \frac{\mu}{[(x - 1 + \mu)^2 + y^2]^{1/2}} = \text{Const.} \quad (3)$$

Auxiliary functions are

$$\left. \begin{aligned} r^2 &= (x + \mu)^2 + y^2, \quad s^2 = (x - 1 + \mu)^2 + y^2 \\ u &= \frac{(1 - \mu)}{r^3}, \quad v = \frac{\mu}{s^3} \end{aligned} \right\} \quad (4)$$

Introducing (4) into (2) transforms (2) into the following second degree system, which can be integrated directly by power series expansions:

$$\left. \begin{aligned} \frac{d^2x}{dt^2} &= x + 2 \frac{dy}{dt} - u(x + \mu) - v(x - 1 + \mu), \quad \frac{d^2y}{dt^2} = y - 2 \frac{dx}{dt} - uy - vy \\ r \frac{du}{dt} + 3u \frac{dr}{dt} &= 0, \quad s \frac{dv}{dt} + 3v \frac{ds}{dt} = 0, \quad r^2 = (x + \mu)^2 + y^2, \quad s^2 = (x - 1 + \mu)^2 + y^2 \end{aligned} \right\} \quad (5)$$

1. The author is very much indebted to Mr. Albert Hirsch, now of the General Electric Co., Phoenix, Arizona, for his extensive and untiring assistance in programming the examples.

2. Cf., for example, Siegel, C. L., Vorlesungen über Himmelsmechanik (Berlin 1956), p. 105.

Let the power series expansion be

$$\left. \begin{aligned} x &= \sum_{\nu=0}^{\infty} X_{\nu} (t-t_0)^{\nu}, \quad y = \sum_{\nu=0}^{\infty} Y_{\nu} (t-t_0)^{\nu} \\ u &= \sum_{\nu=0}^{\infty} U_{\nu} (t-t_0)^{\nu}, \quad v = \sum_{\nu=0}^{\infty} V_{\nu} (t-t_0)^{\nu} \\ r &= \sum_{\nu=0}^{\infty} R_{\nu} (t-t_0)^{\nu}, \quad s = \sum_{\nu=0}^{\infty} S_{\nu} (t-t_0)^{\nu} \end{aligned} \right\} \quad (6)$$

The first coefficients X_0 , X_1 and Y_0 , Y_1 are known at the beginning of the integration step. The first coefficients R_0 , S_0 , U_0 , and V_0 are then determined from (4).

Introducing (6) into (5) and comparing coefficients, we obtain the following recurrence formulas for the succeeding coefficients:

$$\left. \begin{aligned} 2R_0 R_n &= \sum_{\nu=0}^n X_{\nu} X_{n-\nu} + 2\mu X_n + \sum_{\nu=0}^n Y_{\nu} Y_{n-\nu} - \sum_{\nu=1}^{n-1} R_{\nu} R_{n-\nu} \\ 2S_0 S_n &= \sum_{\nu=0}^n X_{\nu} X_{n-\nu} - 2(1-\mu) X_n + \sum_{\nu=0}^n Y_{\nu} Y_{n-\nu} - \sum_{\nu=1}^{n-1} S_{\nu} S_{n-\nu} \\ nR_0 U_n &= -3 \sum_{\nu=1}^n \nu R_{\nu} U_{n-\nu} - \sum_{\nu=1}^{n-1} \nu U_{\nu} R_{n-\nu} \\ nS_0 V_n &= -3 \sum_{\nu=1}^n \nu S_{\nu} V_{n-\nu} - \sum_{\nu=1}^{n-1} \nu V_{\nu} S_{n-\nu} \\ (n+1) nX_{n+1} &= X_{n-1} + 2nY_n - \mu U_{n-1} + (1-\mu) V_{n-1} - \sum_{\nu=0}^{n-1} (U_{\nu} + V_{\nu}) X_{n-1-\nu} \\ (n+1) nY_{n+1} &= Y_{n-1} - 2nX_n - \sum_{\nu=0}^{n-1} (U_{\nu} + V_{\nu}) Y_{n-1-\nu} \end{aligned} \right\} \quad \begin{aligned} &(n = 1, 2, 3, \dots) \\ &(7) \end{aligned}$$

For $n = 1$, the last sum must be omitted for the first four equations (7).

7. As an example of the restricted problem of three bodies, we have computed a periodic orbit of a particle that moves around both the Earth and Moon. The initial values

$$x_0 = 1.2, y_0 = 0, \left(\frac{dx}{dt}\right)_0 = 0, \left(\frac{dy}{dt}\right)_0 = -1.049 \quad \left(\text{for } \mu = \frac{1}{82.45}\right) \quad (8)$$

for this orbit are taken from a paper by R. R. Newton [1]. Among the initial values given in this paper, we have selected those of the orbit coming closest to the Earth. Figure 1 shows this orbit (including a time scale). Every fifth point computed by the power series method is marked. Clearly, numerical integration with a constant step size would have been impossible.

Table 1 shows, for a number of values of t , the step size Δt (determined automatically from the program) for the power series expansion (PSE) method and for the Runge-Kutta-Nyström (RKN) method.

TABLE 1

	$t \approx 0$	$t \approx 1$	$t \approx 1.5$	$t \approx 2$	$t \approx 3$
Δt for PSE	$0.468 \cdot 10^{-1}$	$0.654 \cdot 10^{-1}$	$0.590 \cdot 10^{-2}$	$0.802 \cdot 10^{-1}$	0.205
Δt for RKN	$0.362 \cdot 10^{-3}$	$0.835 \cdot 10^{-3}$	$0.669 \cdot 10^{-4}$	$0.815 \cdot 10^{-3}$	$0.124 \cdot 10^{-2}$

Table 2 shows, for a few values of t , the errors δJ of the Jacobi integral (with respect to its initial value).

TABLE 2

	$t \approx 2$	$t \approx 4$	$t \approx 6$
δJ for PSE	$+0.164 \cdot 10^{-11}$	$+0.169 \cdot 10^{-11}$	$+0.265 \cdot 10^{-11}$
δJ for RKN	$-0.205 \cdot 10^{-11}$	$-0.209 \cdot 10^{-11}$	$+0.285 \cdot 10^{-11}$

Thus, with the same accuracy, it is possible to use a step size for the power series method that is about 100 times as large as for the Runge-Kutta-Nyström method.

A little more than one full orbital period was computed via both methods. Following are the computer running times for $t = 6.25$ (period ≈ 6.19):

PSE: 1.74 minutes (177 integration steps)
RKN: 9.74 minutes (about 16,900 integration steps)

For the same accuracy, computation by the power series method takes only about 18 per cent as long as by the Runge-Kutta-Nyström method.

8. Numerical integration of the restricted problem of three bodies by power series expansions has already been reported in astronomical literature [2, 3]. However, the advantages of the power series method are not fully apparent in these papers, since they concern problems of motion (e.g., periodic trajectories of the Trojan group in the Sun-Jupiter system) that can be integrated with a constant step size for the entire orbit. And indeed this is how these problems were actually integrated by the authors. But then the central difference formulas of Gauss, for example, could have been used just as effectively and, in our opinion, would have required considerably less computer time.

SECTION III. MOTION OF AN ELECTRON IN THE FIELD OF A MAGNETIC DIPOLE

9. The equations of motion are¹

$$\left. \begin{aligned} r^5 \frac{d^2 x}{ds^2} &= (2z^2 - x^2 - y^2) \frac{dy}{ds} - 3yz \frac{dz}{ds} \\ r^5 \frac{d^2 y}{ds^2} &= -(2z^2 - x^2 - y^2) \frac{dx}{ds} + 3xz \frac{dz}{ds} \\ r^5 \frac{d^2 z}{ds^2} &= 3yz \frac{dx}{ds} - 3xz \frac{dy}{ds} \end{aligned} \right\} \quad (9)$$

The magnetic dipole is assumed to be at the origin; the axis of the dipole coincides with the z axis; s = the arc length of the electron path; and r = the distance of the electron from the origin.

The first integrals of the equations of motion are

$$\left(\frac{dx}{ds} \right)^2 + \left(\frac{dy}{ds} \right)^2 + \left(\frac{dz}{ds} \right)^2 = 1 \quad (10)$$

$$x \frac{dy}{ds} - y \frac{dx}{ds} + \frac{(x^2 + y^2)}{r^3} = k = \text{Const.} \quad (11)$$

1. Cf., for example, Störmer, C., The Polar Aurora (Oxford 1955), p. 217.

Auxiliary functions are

$$\left. \begin{aligned} a &= 2z^2 - x^2 - y^2, & b &= 3yz, & c &= 3xz \\ r^2 &= x^2 + y^2 + z^2, & q &= r^5 \end{aligned} \right\} \quad (12)$$

Introducing (12) into (9) yields the second order system

$$\left. \begin{aligned} q \frac{d^2 x}{ds^2} &= a \frac{dy}{ds} - b \frac{dz}{ds} \\ q \frac{d^2 y}{ds^2} &= -a \frac{dx}{ds} + c \frac{dz}{ds} \\ q \frac{d^2 z}{ds^2} &= b \frac{dx}{ds} - c \frac{dy}{ds} \\ r \frac{dq}{ds} &= 5q \frac{dr}{ds} \end{aligned} \right\} \quad (13)$$

Power series expansion of the functions appearing in (12) and (13)

$$\left. \begin{aligned} x &= \sum_{\nu=0}^{\nu} X_{\nu} (t-t_0)^{\nu}, & y &= \sum_{\nu=0}^{\nu} Y_{\nu} (t-t_0)^{\nu}, & z &= \sum_{\nu=0}^{\nu} Z_{\nu} (t-t_0)^{\nu} \\ a &= \sum_{\nu=0}^{\nu} A_{\nu} (t-t_0)^{\nu}, & b &= \sum_{\nu=0}^{\nu} B_{\nu} (t-t_0)^{\nu}, & c &= \sum_{\nu=0}^{\nu} C_{\nu} (t-t_0)^{\nu} \\ r &= \sum_{\nu=0}^{\nu} R_{\nu} (t-t_0)^{\nu}, & q &= \sum_{\nu=0}^{\nu} Q_{\nu} (t-t_0)^{\nu} \end{aligned} \right\} \quad (14)$$

yields the following recurrence formulas for the coefficients of these functions:

$$\left. \begin{aligned} A_n &= 2 \sum_{\nu=0}^n Z_{\nu} Z_{n-\nu} - \sum_{\nu=0}^n X_{\nu} X_{n-\nu} - \sum_{\nu=0}^n Y_{\nu} Y_{n-\nu} \\ B_n &= 3 \sum_{\nu=0}^n Y_{\nu} Z_{n-\nu} \\ C_n &= 3 \sum_{\nu=0}^n X_{\nu} Z_{n-\nu} \end{aligned} \right\} \quad \begin{aligned} &(n = 1, 2, 3, \dots) \\ &(15) \end{aligned}$$

$$\begin{aligned}
2R_0R_n &= \sum_{\nu=0}^n X_\nu X_{n-\nu} + \sum_{\nu=0}^n Y_\nu Y_{n-\nu} + \sum_{\nu=0}^n Z_\nu Z_{n-\nu} - \sum_{\nu=1}^{n-1} R_\nu R_{n-\nu} \\
nR_0Q_n &= 5 \sum_{\nu=1}^n \nu R_\nu Q_{n-\nu} - \sum_{\nu=1}^{n-1} \nu Q_\nu R_{n-\nu} \\
Q_0(n+1) nX_{n+1} &= \sum_{\nu=1}^n \nu Y_\nu A_{n-\nu} - \sum_{\nu=1}^n \nu Z_\nu B_{n-\nu} - \sum_{\nu=1}^{n-1} \nu(\nu+1) X_{\nu+1} Q_{n-\nu} \\
Q_0(n+1) nY_{n+1} &= - \sum_{\nu=1}^n \nu X_\nu A_{n-\nu} + \sum_{\nu=1}^n \nu Z_\nu C_{n-\nu} - \sum_{\nu=1}^{n-1} \nu(\nu+1) Y_{\nu+1} Q_{n-\nu} \\
Q_0(n+1) nZ_{n+1} &= \sum_{\nu=1}^n \nu X_\nu B_{n-\nu} - \sum_{\nu=1}^n \nu Y_\nu C_{n-\nu} - \sum_{\nu=1}^{n-1} \nu(\nu+1) Z_{\nu+1} Q_{n-\nu}
\end{aligned}
\tag{15} \text{ (cont'd)}$$

(n = 1, 2, 3, ...)

The first coefficients X_0 , X_1 , Y_0 , Y_1 , Z_0 , and Z_1 are known at the beginning of the integration step. The first coefficients A_0 , B_0 , C_0 , R_0 , and Q_0 are then determined from (12) and the succeeding coefficients are obtained from (15). For $n = 1$, the last sum must be omitted from the last five equations of (15).

10. Our example of the motion of an electron in the field of a magnetic dipole may have the following initial conditions:

$$x_0 = 0.7, y_0 = 0, z_0 = 0, \left(\frac{dx}{ds}\right)_0 = 0, \left(\frac{dy}{ds}\right)_0 = 0.8, \left(\frac{dz}{ds}\right)_0 = 0.6 \tag{16}$$

Figure 2 shows the projection of the electron path (including an s-scale) in the (x, y)-plane. Again, every fifth point computed by the power series method is marked. This projection gives a good indication of the true path, since the values for z change slowly and remain relatively small (within ± 0.25).

Table 3 shows, for a number of values of s , the step size Δs , which was again determined automatically from the program.

TABLE 3

	$s \approx 0$	$s \approx 2$	$s \approx 4$	$s \approx 6$	$s \approx 8$	$s \approx 10$
Δs for PSE	0.121	$0.220 \cdot 10^{-1}$	$0.819 \cdot 10^{-2}$	$0.980 \cdot 10^{-1}$	0.289	0.386
Δs for RKN	$0.272 \cdot 10^{-3}$	$0.120 \cdot 10^{-3}$	$0.394 \cdot 10^{-4}$	$0.416 \cdot 10^{-3}$	$0.837 \cdot 10^{-3}$	$0.193 \cdot 10^{-3}$

Table 4 shows, for a number of values of s , the errors δi and δk of the first integrals (10) and (11), with respect to their initial values.

TABLE 4

	$s \approx 2$	$s \approx 4$	$s \approx 6$	$s \approx 8$	$s \approx 10$
δi for PSE	$-0.159 \cdot 10^{-11}$	$-0.193 \cdot 10^{-11}$	$-0.366 \cdot 10^{-11}$	$-0.401 \cdot 10^{-11}$	$-0.399 \cdot 10^{-11}$
δi for RKN	$-0.147 \cdot 10^{-11}$	$-0.286 \cdot 10^{-11}$	$-0.439 \cdot 10^{-11}$	$-0.472 \cdot 10^{-11}$	$-0.487 \cdot 10^{-11}$
δk for PSE	$-0.286 \cdot 10^{-12}$	$-0.354 \cdot 10^{-12}$	$-0.766 \cdot 10^{-12}$	$-0.959 \cdot 10^{-12}$	$-0.941 \cdot 10^{-12}$
δk for RKN	$+0.149 \cdot 10^{-11}$	$+0.259 \cdot 10^{-11}$	$+0.399 \cdot 10^{-11}$	$+0.386 \cdot 10^{-11}$	$+0.372 \cdot 10^{-11}$

Thus, with about the same accuracy in the first integrals, the ratio of the step sizes in this example is even more favorable to the power series method.

For both methods, computation was halted as soon as the electron moved a distance of two units from the magnetic dipole. The following computer running times were required:

PSE: 3.71 minutes (204 integration steps)

RKN: 25.70 minutes (about 37,000 integration steps)

Thus computation by the power series method in this example takes only about 14 per cent as long as by the Runge-Kutta-Nyström method.

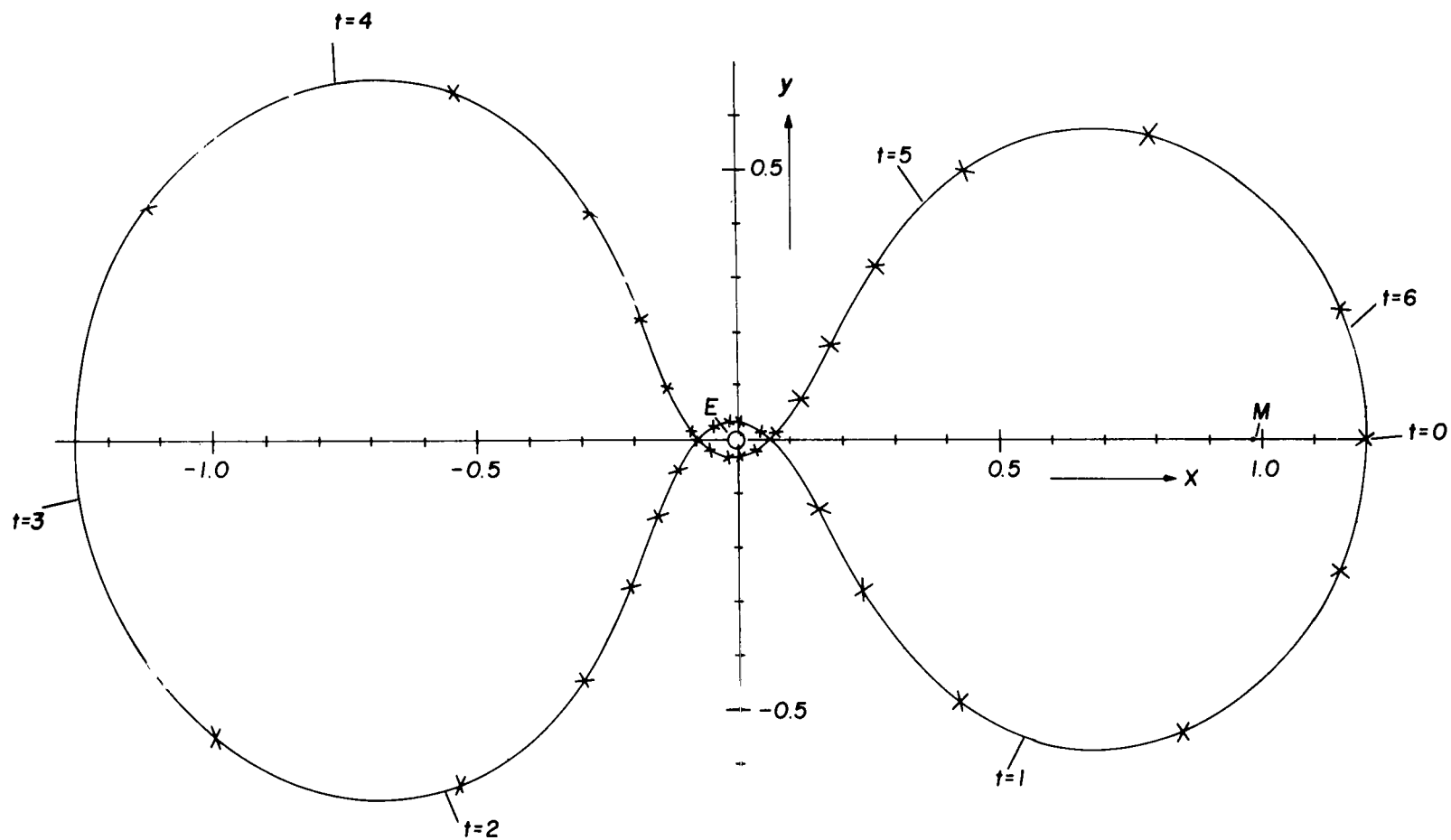


FIGURE 1.

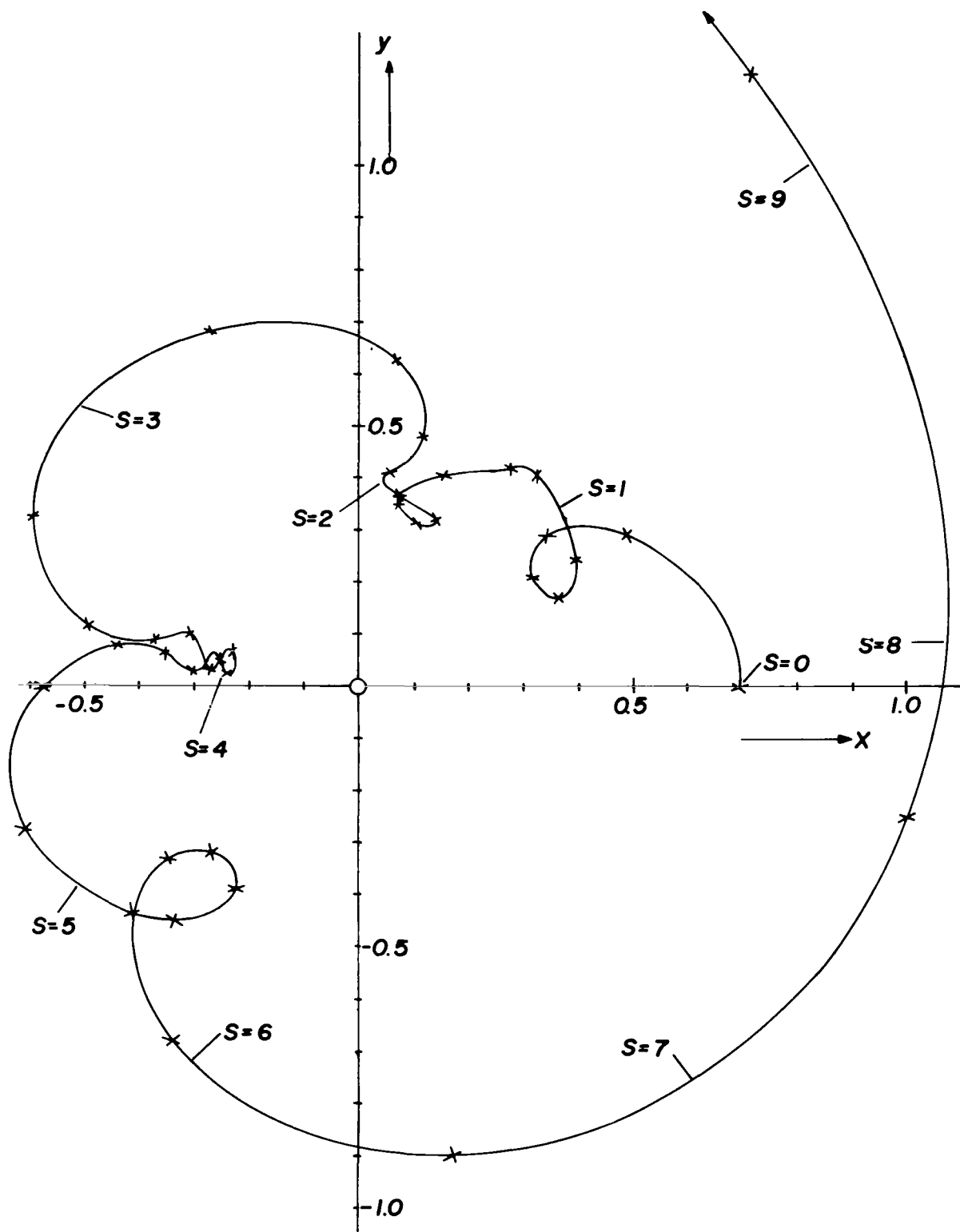


FIGURE 2.

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